WHAT IS CLAIMED AS NEW AND DESIRED TO BE SECURED BY LETTERS PATENT OF UNITED STATES IS:

1. A method for mining mass spectra, comprising:

specifying spectral characteristics of said mass spectra to mine;

specifying a relationship between said spectral characteristics;

searching said mass spectra for portions of said mass spectra which match said spectral characteristics based on said relationship; and

assigning scores to said portions of said mass spectra to indicate a degree of correlation between said portions of said mass spectra and said spectral characteristics.

2. The method of Claim 1, wherein said mass spectra are obtained by any one of dissociation and full-scan.

3. The method of Claim 1, wherein the step of specifying spectral characteristics includes specifying at least one of a product ion, a loss ion, and an ion series.

4. The method of Claim 1, wherein said step of specifying a relationship includes:

identifying each of said spectral characteristics as being one of a primary and a secondary spectral characteristic, said secondary spectral characteristic being linked hierarchically with said primary spectral characteristic and detected only after said primary spectral characteristic is detected.

5. The method of Claim 3, wherein said assigning step includes:

calculating a product ion score;

calculating a loss ion score;

calculating an ion series score;

adjusting said product ion, loss ion, or said ion series score if respective said product ion, loss ion, or ion series spectral characteristic is secondary; and

adding said product ion, loss ion, and ion series scores.

6. The method of Claim 5, wherein the step of calculating a product ion score includes:

identifying a most abundant ion within a window around said product ion spectral characteristic; and

setting said product ion score as a percentage of total ion current of said identified ion.

7. The method of Claim 5, wherein the step of calculating a loss ion score includes:

calculating a loss ion mass per unit charge based on an actual precursor ion mass per unit charge and said loss ion spectral characteristic;

identifying a most abundant ion within a window around said calculated loss ion mass per unit charge; and

setting said loss ion score as a percentage of total ion current of said identified ion.

8. The method of Claim 5, wherein said step of calculating said ion series score includes:

specifying distances between ions in an ion series as the ion series spectral characteristic;

generating hypothetical ions separated by said specified distances;

aligning said mass spectra with said hypothetical ions;

identifying most abundant ions within respective windows around said aligned mass spectra at said specified distances; and

setting said ion series score as a geometric mean of a percentage of total ion current of said identified ions,

wherein said ion series score includes the following term,

$$N\,(I_1 \cdot I_2 \cdot I_3 \ldots \cdot I_n)^{1/n}$$

where N is a number of said identified ions that correspond to said hypothetical ions and $I_1 - I_n$ are respective percentages of said total ion current of said identified ions.

9. The method of Claim 5, wherein said adjusting step includes:

setting said secondary spectral characteristic score as a geometric mean of a primary spectral characteristic score and said secondary spectral characteristic score,

wherein said secondary spectral characteristic score does not exceed said primary spectral characteristic score to which said secondary spectral characteristic score is linked.

10. The method of Claim 1, further comprising:

preprocessing said mass spectra; and

displaying said scores from said assigning step.

11. The method of Claim 10, wherein said preprocessing step includes:

subtracting nonfragment ions from said mass spectra;

estimating precursor charge of mass spectra resulting from said subtracting step; and

normalizing ion intensities of mass spectra from said estimating step as a percentage of a total ion current.

12. The method of Claim 10, wherein the displaying step includes displaying said scores in one of tabular and graphical form.

13. The method of Claim 1, wherein the step of specifying spectral characteristics includes automatically specifying said spectral characteristics based on said mass spectra, and

wherein the step of specifying a relationship includes automatically specifying said relationship based on said mass spectra.

14. The method of Claim 1, further comprising:

adjusting control parameters of a device that produces said mass spectra based on said assigned scores.

15. A method for mining collision-induced dissociation (CID) spectra, comprising:

specifying spectral characteristics of said CID spectra to mine;

specifying a relationship between said spectral characteristics;

searching said CID spectra for portions of said CID spectra which match said spectral characteristics based on said relationship; and

assigning scores to said portions of said CID spectra to indicate a degree of correlation between said portions of said CID spectra and said spectral characteristics.

16. The method of Claim 15, wherein the step of specifying spectral characteristics includes specifying at least one of a product ion, a loss ion, and an ion series.

17. The method of Claim 15, wherein said step of specifying a relationship includes:

identifying each of said spectral characteristics as being one of a primary and a secondary spectral characteristic, said secondary spectral characteristic being linked hierarchically with said primary spectral characteristic and detected only after said primary spectral characteristic is detected.

18. The method of Claim 16, wherein said assigning step includes:

calculating a product ion score;

calculating a loss ion score;

calculating an ion series score;

adjusting said product ion, loss ion, or said ion series score if respective said product ion, loss ion, or ion series spectral characteristic is secondary; and

adding said product ion, loss ion, and ion series scores.

19. The method of Claim 18, wherein the step of calculating a product ion score includes:

identifying a most abundant ion within a window around said product ion spectral characteristic; and

setting said product ion score as a percentage of total ion current of said identified ion.

20. The method of Claim 18, wherein the step of calculating a loss ion score includes:

calculating a loss ion mass per unit charge based on an actual precursor ion mass per unit charge and said loss ion spectral characteristic;

identifying a most abundant ion within a window around said calculated loss ion mass per unit charge; and

setting said loss ion score as a percentage of total ion current of said identified ion.

21. The method of Claim 18, wherein said step of calculating said ion series score includes:

specifying distances between ions in an ion series as the ion series spectral characteristic;

generating hypothetical ions separated by said specified distances;

aligning said CID spectra with said hypothetical ions;

identifying most abundant ions within respective windows around said aligned CID spectra at said specified distances; and

setting said ion series score as a geometric mean of a percentage of total ion current of said identified ions,

wherein said ion series score includes the following term,

$$N\,(I_1 \cdot I_2 \cdot I_3 \ldots \cdot I_n)^{1/n}$$

where N is a number of said identified ions that correspond to said hypothetical ions and $I_1 - I_n$ are respective percentages of said total ion current of said identified ions.

22. The method of Claim 18, wherein said adjusting step includes:

setting said secondary spectral characteristic score as a geometric mean of a primary spectral characteristic score and said secondary spectral characteristic score,

wherein said secondary spectral characteristic score does not exceed said primary spectral characteristic score to which said secondary spectral characteristic score is linked.

23. The method of Claim 15, further comprising:

preprocessing said CID spectra; and

displaying said scores from said assigning step.

24. The method of Claim 23, wherein said preprocessing step includes:

subtracting nonfragment ions from said CID spectra;

estimating precursor charge of CID spectra resulting from said subtracting step; and

normalizing ion intensities of CID spectra from said estimating step as a percentage of a total ion current.

25. The method of Claim 23, wherein the displaying step includes displaying said scores in one of tabular and graphical form.

26. The method of Claim 15, wherein the step of specifying spectral characteristics includes automatically specifying said spectral characteristics based on said CID spectra, and

wherein the step of specifying a relationship includes automatically specifying said relationship based on said CID spectra.

27. The method of Claim 15, further comprising:

adjusting control parameters of a device that produces said CID spectra based on said assigned scores.

28. A system for mining mass spectra, comprising:

means for specifying spectral characteristics of said mass spectra to mine;

means for specifying a relationship between said spectral characteristics;

means for searching said mass spectra for portions of said mass spectra which match said spectral characteristics based on said relationship; and

means for assigning scores to said portions of said mass spectra to indicate a degree of correlation between said portions of said mass spectra and said spectral characteristics.

29. The system of Claim 28, wherein said mass spectra are obtained by any one of dissociation and full-scan.

30. The system of Claim 28, further comprising:

means for preprocessing said mass spectra; and

means for displaying said scores from said assigning means.

31. The system of Claim 28, wherein the means for specifying spectral characteristics includes means for automatically specifying said spectral characteristics based on said mass spectra, and

wherein the means for specifying a relationship includes means for automatically specifying said relationship based on said mass spectra.

32. The system of Claim 28, further comprising:

means for adjusting control parameters of a device that produces said mass spectra based on said assigned scores.

33. A system comprising:

a memory device having embodied therein mass spectra; and

a processor in communication with the memory device, the processor configured to

specify spectral characteristics of said mass spectra to identify,

specify a relationship between said spectral characteristics,

search said mass spectra for portions of said mass spectra which match said spectral characteristics based on said relationship, and

assign scores to said portions of said mass spectra to indicate a degree of correlation between said portions of said mass spectra and said spectral characteristics.

34. A computer program product including a computer readable medium for mining mass spectra, comprising:

a graphical user interface code configured to allow a user to input spectral characteristics to mine and specify a relationship between said spectral characteristics; and

a mining code configured to search said mass spectra for portions of said mass spectra matching said spectral characteristics based on said relationship and assign scores to said portions of said mass spectra to indicate a degree of correlation between said portions of said mass spectra and said spectral characteristics.

35. The computer program product of Claim 34, wherein said mass spectra are obtained by any one of dissociation and full-scan.

36. The computer program product of Claim 34, wherein the graphical user interface code is configured to accept at least one of a product ion, a loss ion, and an ion series as an input,

identify said spectral characteristics as being one of a primary and a secondary spectral characteristic, and

link said secondary spectral characteristic with said primary spectral characteristic such that said secondary spectral characteristic is detected only after said primary spectral characteristic is detected.

37. The computer program product of Claim 34, wherein the graphical user interface code comprises:

a control window configured to input the spectral characteristics and the relationship between said spectral characteristics of said mass spectra; and

a results window configured to display said scores of said mass spectra.

38. The computer program product of Claim 36, wherein the mining code is configured to

calculate a product ion score,

calculate a loss ion score,

calculate an ion series score,

adjust said product ion, loss ion, or said ion series score if respective said product ion, loss ion, or ion series spectral characteristic is secondary, wherein said secondary spectral characteristic score does not exceed said primary spectral characteristic score to which said secondary spectral characteristic score is linked, and

add said product ion, loss ion, and ion series scores.

39. The computer program product of Claim 38, wherein said mining code is further configured to

calculate the product ion score by identifying a most abundant ion within a window around said product ion spectral characteristic and setting said product ion score as a percentage of total ion current of said identified ion,

calculate the loss ion score by calculating a loss ion mass per unit charge based on an actual precursor ion mass per unit charge and said loss ion spectral characteristic, identifying a most abundant ion within a window around said calculated loss ion mass per unit charge, and setting said loss ion score as a percentage of total ion current of said identified ion, and

calculate the ion series score by specifying distances between ions in an ion series as the ion series spectral characteristic, generating hypothetical ions separated by said specified distances, aligning said mass spectra with said hypothetical ions, identifying most abundant ions within respective windows around said aligned mass spectra at said specified distances, and setting said ion series score as a geometric mean of a percentage of total ion current of said identified ions,

wherein said ion series score includes the following term,

$$N\,(I_1 \cdot I_2 \cdot I_3 \ldots \cdot I_n)^{1/n}$$

where N is a number of said identified ions that correspond to said hypothetical ions and $I_1 - I_n$ are respective percentages of said total ion current of said identified ions.

40. The computer program product of Claim 34, further comprising:

a preprocessing code configured to process said mass spectra prior to mining in order to remove spurious mass spectra.

41. The computer program product of Claim 40, wherein the preprocessing code is configured to

subtract nonfragment ions from said mass spectra,

estimate precursor charge of mass spectra resulting from said subtracting step, and

normalize ion intensities of mass spectra from said estimating step as a percentage of a total ion current.

42. The computer program product of Claim 37, wherein the graphical user interface code further comprises:

a product ion window configured to input said product ion spectral characteristic;

a loss ion window configured to input said loss ion spectral characteristic; and

an ion series window configured to input said ion series spectral characteristic,

wherein said product ion, loss ion, and ion series windows open when respective said spectral characteristics are selected in said control window.

43. The computer program product of Claim 37, wherein said results window displays said scores in one of tabular and graphical form.

44. The computer program product of Claim 34, wherein the graphical user interface code is configured to accept automatically specified said spectral characteristics and said relationship based on said mass spectra.

45. The computer program product of Claim 34, further comprising:

a control code configured to adjust control parameters of a device which generates said mass spectra based on said assigned scores.

46. A computer readable medium containing program instructions for execution on a computer system, which when executed by the computer system, cause the computer system to perform the method recited in any one of claims 1 through 14.

47. A graphical user interface, comprising:

a control window configured to input spectral characteristics and a relationship between said spectral characteristics of mass spectra; and

a results window configured to display scores of said mass spectra indicating how well said mass spectra match said spectral characteristics.

48. The graphical user interface of Claim 47, wherein said results window displays said scores in one of tabular and graphical form.